Theory of Condensed Matter Group Scientific Meeting

University of Warwick, Tuesday 6th June 2017

10.30 Arrival and Coffee

11.00 **Nicholas Bristowe**, Kent
First principles and group theoretical design of magnetoelectric multiferroics

11.50 **Rebecca Nicholls**, Oxford
Enhancing materials design using microscopy and modeling

12.40 Lunch

13.40 **Tapio Ala-Nissila,** Aalto/Loughborough
Tension propagation theory and its application to polymer driven translocation

14.30 Posters (including student poster prize) with tea at 15.30

16.10 **Andrew James**, UCL
Time-dependent behaviour in 2D many-body systems: combining exact solutions and matrix-product states

17.00 Close

The meeting will be held off the Warwick Science Concourse.
The ordering of speakers is subject to revision.

Organised by Andrew Morris, *Cambridge*, Halim Kusumaatmaja, *Durham,* Nicholas d'Ambrumenil, *Warwick*

Registration + further details: theory.warwick.ac.uk/events/iop2017

IOP Institute of Physics
Theory of Condensed Matter Group

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Posters

1. Jason Lewis and Matthew Turner, *Warwick*, Density regulation in models of metric-free swarms
2. Ehren Mellars and Benjamin Béri, *Birmingham*, Signatures of time-reversal-invariant topological superconductivity in the Josephson effect
3. Josef Oswald and Rudolf Roemer, *Leoben/Warwick*, Exchange-mediated screening in the integer quantum Hall effect
   We study many-body interaction effects in the spatially resolved filling factor (ν) distribution for higher Landau levels (LLs) via self-consistent Hartree-Fock simulations in the integer quantum Hall (IQH) regime. Our results indicate a strong, interaction-induced tendency to avoid the simultaneous existence of partially filled spin-up and spin-down LLs. Rather, we find that such partially filled LLs consist of coexisting regions of full and empty LLs. At the boundaries between the regions of full and empty LLs, we observe edge stripes of nearly constant ν close to *half-filling*. This suggests that the exchange interaction induces a behavior similar to a Hund's rule for the occupation of the spin split LLs. The screening of the disorder and edge potential appears significantly reduced as compared to static Thomas-Fermi screening (Chklovskii D. B. *et al.*, *Phys. Rev. B*, **46** (1992) 4026). Our results are consistent with a local, lateral ν-dependence of the exchange-enhanced spin splitting. Hence, on quantum-coherent length scales as probed here, the electron system of the IQH effect behaves similarly to a non-interacting single particle system —not because of the absence, but rather due to the dominance of many-body effects
4. J.P. Hague and C. MacCormick. *Open University*, Implementation strategies for multiband quantum simulators of real materials
5. Oliver T. Dyer and Robin C. Ball, *Warwick*, Wavelet Monte Carlo dynamics: hydrodynamics without the calculation
6. M. Offidani, F. Sousa, and A. Ferreira , *York*, Theory of charge-spin interconversion in 2D Dirac-Rashba models
7. Stela Makri, James Kermode and Christoph Ortner, *Warwick Centre for Predictive Modelling*
8. A.A. Tomlinson and N.K. Wilkin, *Birmingham*, Observation of Chaos in a Constricted Vortex Flow Channel
9. S. C. Al-Izzi, G. Rowlands, P. Sens and M. S. Turner, *Warwick*, Osmotic effects on organelle biogenesis
10. Manjinder Kainth and Martin Long, *Birmingham*, Superconductivity Mediated By a Strong Hubbard Repulsion
11. Antonino Savojardo, Marc Eberhard, Rudolf Roemer, *Warwick/Aston*, Roguewave generation by inelastic quasi-soliton collisions in optical fibres
    Optical rogue waves are sharp, rare and extremely high power pulses. We demonstrate that such waves can be generate by a simple cascade mechanism based on inelastic collisions of quasi-solitons. The mechanism exploits the fact that pulses are well localized inside an optical fiber and interact in pairs. Based on statistics from more than $17 \cdot 10^6$ pulses, we establish unambiguously the long-tail character of the probability distribution function (PDF). Time series

analysis of such rogue waves shows a typical signature of few picoseconds, opening the possibility of predicting them before they pass.

12. Joseph C.A. Prentice, Bartomeu Monserrat, Richard J. Needs, *Cambridge*, First-principles anharmonic calculations and the dynamic Jahn-Teller effect

13. J. Gartlan and N. Wilkin, *Birmingham,*
We have numerically shown that the minimum energy solution of repulsive particles in a gravitational field is an arc-like conformal lattice which has height dependent density, this structure can also be obtained by applying a conformal mapping to the hexagonal lattice. The arc-like structure is resilient to small changes in the particle number, width and applied temperature. When varying the intensity of the gravitational field we observe a sharp Kosterlitz-Thouless transition. The hexatic order of the system also shows some unusual features as the penetration depth is varied.

14. Simon Malzard, Charles Poli and Henning Schomerus, *Lancaster*, Emergent charge-conjugation symmetry and topologically protected defect states in lossy photonic systems

15. R Roemer and E R Matamero, Warwick, The dynamics and flexibility of biomedically important proteins
700,000 people die each year from drug-resistant infections, a figure that - if action is not taken - is estimated to increase to 10 million by 2050. The drug penicillin targets essential cell wall biosynthetic enzymes that still remain attractive targets for new efforts in drug discovery. Elucidating protein dynamics and flexibility is key to understaning the selective interactions of proteins with a drug as it docks. In spite of the success of x-ray crystallography in the determination of rigid protein structures, the experimental technique is unable to provide insight into the dynamics and flexibility of proteins. Such information can, however, be elucidated using molecular modelling. Important protein conformational changes often occur on microsecond-millisecond timescales and are difficult to access using traditional modelling techniques, such as molecular dynamics (MD). Here, we present the method and results of computationally inexpensive, geometric simulations of protein motion for a range of proteins important in antimicrobial resistance (AMR).

16. Stephen Spurrier and Nigel R. Cooper, *Cambridge*, Semiclassical Dynamics and Berry Curvature in Optical Quasicrystals

17. Edoardo G. Carnio, Nicholas D. M. Hine, Rudolf A. Römer, *Warwick*, The Anderson transition in doped silicon using *ab initio* methods
The Anderson localisation-delocalisation transition (AT) has long been studied using paradigmatic models, but there is still no agreement on its critical exponent when comparing experiments and theory. In this work, we employ *ab initio* methods to study the AT occurring in sulfur-doped silicon (Si:S) when increasing the dopant concentration. We use ONETEP, a linear-scaling implementation of DFT, to study model Si:S systems with few impurities, and we subsequently employ the resulting *ab initio* Hamiltonians to build an effective tight-binding model for systems close to the critical concentration of the AT. We observe the formation of an impurity band, compute its density of state, and apply multifractal finite-size scaling of the wave functions to characterise the transition.

18. Mark Skelton, *Warwick,* How does a Bohm particle localize?
At present, we are making little progress in finding a theory which would unify gravity and quantum physics. Some propose that this is due to an incomplete

understanding of quantum physics, or more precisely that the Copenhagen interpretation of quantum mechanics is inadequate. One alternative interpretation is de Broglie-Bohm theory, and this project will focus on Anderson Localization and reinterpret it in the context of this theory. Specifically, we will study the trajectories of Bohm particles for wave packets in the localized, critical and diffusive phases. The theory will be checked by computer simulations which track the trajectories of Bohm particles, to study how spatial localization and multifractality occur with- out contradictions, for example if the Bohm trajectories cross paths or if they enter nodal regions of the wave function. The trajectories produced from this simulation will be used to study some semi-classical characteris- tics such as scar states, and in addition their variation with magnetic flux will be studied. In the case of a fully localized one-dimensional disordered chain, by treating the trajectories as in standard non-linear dynamics their Lyapunov exponents, if they exist, will be measured.

19. Andrew Hallam, Andrew James and Andrew Green, *UCL*, Quantum quenches in two spatial dimensions